

Multidimensional tunneling between potential wells at non degenerate minima

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We consider tunneling between symmetric wells for a 2-D semi-classical Schrödinger operator for energies close to the quadratic minimum of the potential V in two cases: (1) excitations of the lowest frequency in the harmonic oscillator approximation of V ; (2) more general excited states from Diophantine tori with comparable quantum numbers.

1 TUNNELING BETWEEN DOUBLE WELLS: A SHORT REVIEW

Tunneling for Schrödinger type operators involves various scenarios which depend on the details of the dynamics, ranging from integrable or quasi-integrable systems, to ergodic or chaotic ones.

Assume that V is a smooth function, symmetric with respect to $\{x_1 = 0\}$, and $\{V(x) \leq E\}$ consists in 2 connected components $(U_E)_{L/R}$ (the potential wells), while $\limsup_{|x| \rightarrow \infty} V > E$. We are interested in the semi-classical spectrum of Schrödinger operator $P = -\hbar^2 \Delta + V$ on $L^2(\mathbf{R}^2)$ near energy E , which consists in pairs $E^\pm(h) = E_k^\pm(h)$ exponentially close to eigenvalues $E(h) = E_k(h)$ of the Dirichlet realization of P in some neighborhood of a single well. We will always assume ([14],[15]) that $E(h)$ are simple (non degenerate) and asymptotically simple. As a general rule, the energy shift $\Delta E(h) = E^+(h) - E^-(h)$ (or splitting of eigenvalues) is related to so called Agmon distance $S(E)$ between the wells, associated with the degenerate, conformal metric $ds^2 = (V - E)_+ dx^2$ that measures the life-span of the particle in the classically forbidden region $V(x) \geq E$. Much is known in the 1-D case, even for excited states, or in several dimensions for the lowest eigenvalues.

At the higher level of generality, we only require that $V'(x) \neq 0$ on $\{V = E\} = \partial U_L(E) \cup \partial U_R(E)$. In the 1-D case, Landau-Lifshitz formula reads

$$\Delta E(h) = 2 \frac{\omega h}{\pi} e^{-S(E)/h} (1 + o(1)) \quad (1)$$

where $\omega = \frac{\partial p}{\partial I}$ is the frequency of the periodic orbit at energy E , and $2S(E) = I = 2\pi^{-1} \oint (E - V)_+ dx$. In higher dimensions, the structure of the classical flow plays an essential rôle, so that we are left with the following equivalence (see [15] for a precise statement): Assume V is analytic. Then the splitting $\Delta E(h)$ is non exponentially small with respect to Agmon distance (i.e. for all $\varepsilon > 0$, larger than a constant times $e^{-(S(E)+\varepsilon)/h}$, $0 < h \leq h_\varepsilon$) iff the eigenfunctions of P , with eigenvalues $E^\pm(h)$, are non exponentially small (i.e. for all $\varepsilon > 0$, larger, in local L^2 norm, than a constant times $e^{-\varepsilon/h}$, $0 < h \leq h_\varepsilon$) in an open set where minimal geodesics, connecting the 2 wells, meet their boundary. These propositions are true for instance when the flow is ergodic inside the wells, and false in case of separation of variables (complete integrability).

Here we are interested in the special case of “tunnel cycles” for quasi-integrable flows, for which propositions hold true. Let V have non degenerate minima $a_{L/R}$ with $V(a_{L/R}) = 0$, and $V_0 = \sum_j \lambda_j^2 z_j^2$, $\lambda_1 < \lambda_2$ be the harmonic approximation (in local coordinates z) around $a_{L/R}$ and $p_0(x, \xi) = \xi^2 + V_0$, the quadratic part of $p(x, \xi)$ near 0.

In 1-D the splitting between the lowest eigenvalues is found to be

$$\Delta E(h) = 2 \sqrt{\frac{\pi \omega h}{e}} \frac{\omega h}{\pi} e^{-S_h/h} (1 + o(1)) \quad (2)$$

$\omega = \lambda_1$ is the harmonic frequency, and S_h half the action of the periodic orbit for the Hamiltonian with reversed potential $q = \xi^2 - V$ at energy $-E$, $E = \omega h/2$. For higher energies we have

$$\Delta E_m(h) = 2b_m \frac{\omega h}{\pi} e^{-S(E)/h} (1 + o(1)),$$

where

$$E = (2m+1)\omega h, \quad b_m = \frac{\sqrt{\pi}(2m+1)^{m+1/2}}{2^m m! e^{m+1/2}} \quad (3)$$

so long $mh \leq c$, $c > 0$ small enough, which somehow “interpolates” between (??) and (??) since $b_m \rightarrow 1$ as $m \rightarrow \infty$.

In several dimensions, the splitting between the two lowest eigenvalues [6],[1],[2] is again of the form

$$\Delta E(h) = 2\sqrt{\frac{\pi}{e}} \frac{\lambda_1 h}{\pi} e^{-S_h/h} (1 + o(1))$$

Further, such formulas hold between any *low-lying eigenvalues*, i.e. for any N , there is $h_N > 0$ such that for each principal quantum number $m \leq N$, the splitting $\Delta E_m(h)$ has an asymptotic of the form $\Delta E_m(h) \sim a_m(h) e^{-S_h/h}$ provided $0 < h < h_N$ [11], [14]. See also [16] for degenerate minima.

In this report we restrict our attention to KAM states, i.e. supported near a Diophantine torus and with quantum numbers (k_1, k_2) such that $|k|h \leq c$, or semi-excited states in the limit $c \rightarrow 0$, i.e. when $|k| \rightarrow \infty$ and $h \rightarrow 0$ are related by $|k|h \leq h^\delta$, $0 < \delta < 1$. Further we shall only consider states (or approximate eigenfunctions) microlocalized on isotropic (generally Lagrangian) manifolds whose analytic continuation in the momentum space (i.e. in the classically forbidden region) are in a generic position. Lagrangian manifolds of 2 types are relevant to our analysis: (1) the flow-out of the boundary of the wells (2) the quasi-invariant tori making a local fibration of the energy surface inside the wells. They have a (singular) limit as $E \rightarrow 0$.

2 ENERGY SURFACES AND LIBRATIONS

The Lagrangian manifolds of the first type are the integral manifold of q passing above $(\partial U_E)_{L/R}$. From now on we assume that in local coordinates near $a_{L/R}$, $p(x, \xi) = p_0(x, \xi) + \mathcal{O}(|z|^3)$. Consider first a single well U_E then locally

$$\Lambda_\partial^E = \{\exp t H_q(\rho) : \rho \in \partial U_E \times 0, q(\rho) = -E, t \in \mathbf{R}\}$$

is a smooth real Lagrangian submanifold of the form $\xi = \pm \nabla d_E(x)$, $x \notin U_E$, with a fold along ∂U_E . Here $d_E(x) = d_E(x, \partial U_E)$ is Agmon distance from x to ∂U_E and satisfies (locally) the eikonal equation $(\nabla d_E(x))^2 = V(x) - E$. As $E \rightarrow 0$, Λ_∂^E tends to the union of the outgoing/incoming Lagrangian manifolds Λ^\pm (called separatrices in 1-D) with a conical intersection at the origin.

We shall assume that $(\Lambda_\partial^E)_{L/R}$, as integral manifolds of Hamiltonian flow, extend away from the wells as Lagrangian manifolds intersecting in the energy surface $\{q(\rho) = -E\}$ along a curve γ_E .

This curve projects onto \mathbf{R}_x^2 precisely as a *libration* Lib_E between $U_L(E)$ and $U_R(E)$, i.e. a periodic orbit with end points at $\partial U_{L/R}(E)$ [3]. We assume for simplicity there is exactly one such family of curves. We call also Lib_E a *minimal geodesic* between $U_L(E)$ and $U_R(E)$ for Agmon distance $ds^2 = \sqrt{(V(x) - E)_+} dx^2$. Assuming PT symmetry (i.e. V symmetric with respect to $\{x_1 = 0\}$), we denote by $\{x_E\} = \text{Lib}_E \cap \{x_1 = 0\}$. Then $d_E(x_E, U_L^E) = d_E(x_E, U_R^E) = S_E/2$, and Lib_E intersects $\{x_1 = 0\}$ at x_E with a right angle. A neighborhood of x_E in $\{x_1 = 0\}$ can be thought of as Poincaré section, intersecting γ_E transversally. The γ_E are (unstable) periodic orbits of hyperbolic type, with real Floquet exponent $\beta(E)$. Of course, because of focal points, $(\Lambda_\partial^E)_{L/R}$ doesn’t extend smoothly everywhere but only in a neighborhood of librations when the system is not integrable.

As $E \rightarrow 0$ the libration degenerates to an *instanton* γ_0 . Parametrized as a bicharacteristic of $q(x, \xi)$ at $E = 0$, it takes an infinite time to reach the equilibria a_L or a_R along γ_0 . We shall assume that the stable outgoing and incoming manifolds $\Lambda_{L/R}^\pm$ at 0 intersect transversally at γ_0 .

3 QUASI-INVARIANT LIOUVILLE TORI

Lagrangian manifolds of the second type are the invariant tori foliating (locally) the energy surface in the integrable case, or KAM tori, or corresponding quasi-invariant tori in the quasi-integrable case. In the Section 6, we shall also allow these Lagrangian manifolds to shrink to periodic orbits.

We can have already a good insight into the problem in replacing V by its quadratic approximation. This is what we call the *model case*. When frequencies λ_j are rationally independent, we can essentially reduce to the model case by resorting to Birkhoff normal forms (or KAM theorem).

So assume for simplicity that $p = p_0$ near $a_{L/R}$. Then for small $E > 0$, the energy surfaces are foliated by invariant tori Λ_i , $E = 2\lambda_1 \iota_1 + 2\lambda_2 \iota_2$ which can be extended in the complex domain along complex times, e.g. as integral leaves $\tilde{\Lambda}_i$ of $q(x, \xi) = \xi^2 - \lambda_1^2 z_1^2 - \lambda_2^2 z_2^2$, with purely imaginary time.

The caustics of Λ_i can be viewed as a rectangle shaped fold line delimiting the zone of pure oscillations of the quasi-modes, and touching the boundary of the wells ∂U_E , $E = 2\lambda_1 \iota_1 + 2\lambda_2 \iota_2$ at 4 vertices, the hyperbolic umbilic points (HU) points, section of the torus by the plane $\xi = 0$ in \mathbf{R}^4 . We

Definition 2 The action $\int_{\tilde{y}(y_L)}^{\tilde{y}(y_R)} \xi dx$ computed on $\tilde{\gamma}(y)$ is called the tunnel distance between $(\Lambda_{\iota(y)})_L$ and $(\Lambda_{\iota(y)})_R$ (it equals Agmon distance when $\tilde{\gamma}(y) = \gamma_E$.)

Let $y \in \partial_E(y)$. Integrating ξdx along γ_y gives (locally) Agmon distance to the well :

$$d_E(x) = \int_y^x \xi dx = \sum_j \lambda_j \int_{y_j}^{x_j} \sqrt{t^2 - y_j^2} dt, \quad x \in \gamma_y$$

Denote by $F_y^E(x)$ the RHS of this equation; provided $y \in \partial U_E$ is not too close to both z -axis, one can show that $F_y^E(x) - d_E(x)$ is estimated by the square of the (Euclidean) distance of x to its orthogonal projection on γ_y , for x in a neighborhood of Lib_E . Similarly we consider variations from the regular part of the caustics $\mathcal{C}(y) \inf\{\int_0^1 (V(\gamma(s)) - E)_+^{1/2} |\dot{\gamma}(s)| ds, \text{ with } (\gamma(0), \dot{\gamma}(0)) \in T\mathcal{C}(y), \gamma(1) = x, \text{ and write the critical value as } G_{\mathcal{C}(y)}^E(x) = \int_{\tilde{y}(x)}^x \xi dx, \text{ or simply } G_{\mathcal{C}(y)}^E(x) = \int_{\mathcal{C}(y)}^x \xi dx. \text{ Again } G_{\mathcal{C}(y)}^E(x) - d_E(x) + \int_y^{\tilde{y}(x)} \xi dx = F_y^E(x) - d_E(x), \text{ where } \int_y^{\tilde{y}(x)} \xi dx, \tilde{y}(x) \in \mathcal{C}(y) \text{ is a small error term essentially independent of } x \text{ in a neighborhood of } \text{Lib}_E.$

The next step consists in constructing quasi-modes. First we construct quasi-modes microlocalized on the Λ_ι selecting a sequence $\iota = \iota_k(h)$ from Bohr-Sommerfeld-Maslov (or EBK) quantization rules. As a rule, these (oscillating) quasi-modes extend in the shadow zone near $y_k(h)$ with exponential decay. They can further be extended to u_L and u_R along $\tilde{\gamma}(y_k(h))$ using WKB expansions, or the ‘‘Gaussian beams’’ method. The eigenvalue splitting is given by the usual formula

$$\Delta E_k(h) \sim 4h^2 \int_{\Sigma} u_L(0, x_2) \frac{\partial u_R}{\partial x_1}(0, x_2) dx_2 \quad (6)$$

where Σ is a neighborhood of x_E in $\{x_1 = 0\}$. We now treat some specific cases in more detail.

5 TUNNELING NEAR A PAIR OF DIOPHANTINE TORI

Assume $c > 0$ is so small that KAM theory ensures existence of a family invariant tori in the well $U_E = U_L(E)$ for $E \leq c$. We are interested in $\Delta E_k(y)$ for $E_k(h)$ near such fixed $E > 0$. Assume that Lib_E starts at umbilic y_E away from the z -axis, and for simplicity, that $y_E \in \Lambda_\iota$ with ι in

the KAM set, i.e. such that the motion on Λ_ι is quasi-periodic with Diophantine frequency vector ω (this assumption seems to be generic, varying slightly E). In [8], we proved the following : Let $0 < \delta < 1$. Then in a $h^{\delta/2}$ -neighborhood of Λ_ι in T^*M , there is a family Λ_J of tori, labelled by their action variables $J = J_k(h)$ for $k \in \mathbf{Z}^d$ satisfying $|kh - \iota| \leq h^\delta$, which verify Bohr-Sommerfeld-Maslov quantization condition, and are quasi-invariant under H_p with an accuracy $\mathcal{O}(h^\infty)$. At first approximation, the umbilics $y_k(h) \in \Lambda_J$ have the form $y \sim (\lambda_1^{-1} \sqrt{2\lambda_1 \iota_1}, \lambda_2^{-1} \sqrt{2\lambda_2 \iota_2})$ or $y \sim (\lambda_1^{-1} \sqrt{2h\lambda_1 k_1}, \lambda_2^{-1} \sqrt{2h\lambda_2 k_2})$, $k = (k_1, k_2) = k(h) \in \mathbf{N}^2$ so the typical neighboring distance between $y_k(h)$ is $hE^{-1/2}$ when y_E stays away from the z -axis. Using Maslov canonical operator, we obtain from these tori a sequence of quasi-modes for P near E . By complex contour integrals ([9], [12]) they extend in a $|h \log h|^{2/3}$ -neighborhood of U_E , as states microlocalized on $\tilde{\Lambda}_J$, and decaying exponentially as $\exp[-F_y^E(x)/h]$, or $\exp[-G_{\mathcal{C}(y)}^E(x)/h]$. This decay propagates all along $\tilde{\gamma}(y_k(h))$ and nearby bicharacteristics, which stay in the purely decaying branch $\tilde{\Lambda}_J$ of Λ_J .

Next we need to compare the tunnel distance with Agmon distance which coincide only on the tunnel cycle. Let $S_L - S_R$ be the tunnel action between y_L and y_R , we have at $\{x_1 = 0\}$ (see Fig.1)

$$\begin{aligned} S_L - S_R - 2S_0(E) &= 2(F_y^{E(y)}(\tilde{x}(y)) - d_{E(y)}(\tilde{x}(y))) \\ &\quad + 2(d_{E(y)}(\tilde{x}(y)) - d_E(\tilde{x}(y))) \\ &\quad + 2(d_E(\tilde{x}(y)) - d_E(x_E)) \end{aligned} \quad (7)$$

Evaluating each error term on the RHS, we arrive at $S_L - S_R - 2S_0(E) = o(1)$, $h \rightarrow 0$. Then $S_L - S_R$ has a non degenerate critical point at $\tilde{x}(y_k(h))$ belonging to the tunnel bicharacteristic $\tilde{\gamma}(y_k(h))$ common to $(\tilde{\Lambda}_{J_k(h)})_L$ and $(\tilde{\Lambda}_{J_k(h)})_R$. The integral can be computed by standard stationary phase expansion around $x_k(h)$. Since the amplitude of u_R (and u_L) is non vanishing, we obtain eventually [5]

$$\Delta E_k(h) \sim B_k(h) e^{-(S_L - S_R)/h}$$

with $B_k(h) \sim \frac{h^{3/2}}{\sqrt{\tau_L \sigma(H_L, H_R) \tau_R}}$. Here $H_{L/R}$ are Hamilton vector fields tranverse to γ_E , and $\tau_{L/R}$ suitable Jacobians computed on $(\tilde{\Lambda}_{J_k(h)})_{L/R}$.

6 THE QUASI 1-D CASE

In this section we shall assume that frequencies λ_1, λ_2 are non-resonant, with $2\lambda_1 < \lambda_2$, and the

instanton γ_0 approaches the node singularity of the outgoing and incoming manifolds $\Lambda_{L/R}^\pm$ at $a_{L/R}$ in a regular direction (associated with λ_1). We consider eigenstates with quantum vector $(m, 0)$ for $m \in \mathbb{N}$, i.e. $E_m = h(\lambda_1(2m+1) + \lambda_2) + \mathcal{O}(h^2)$, and compute asymptotics for the energy splitting ΔE_m (as $h \rightarrow 0$, while m stays fixed, and probably also when $hm \leq h^\delta$, $0 < h < 1$.) This amounts to let Λ_ϵ shrink to an isotropic torus.

Theorem 1 *Under the assumptions above*

$$\Delta E_m = 2b_m \frac{\omega_1 h}{\pi} e^{-\frac{S(\tilde{E})}{h}} (1 + o(1)), \quad h \rightarrow 0,$$

where b_m is found from (??), $S(\tilde{E})$ is half the action on $\text{Lib}_{\tilde{E}}$ at energy $\tilde{E} = \tilde{E}(h)$ which we determine as the solution of:

$$\tilde{E} + h\beta(\tilde{E}) = h(\lambda_1(1+2m) + \lambda_2). \quad (8)$$

Here $\beta(\tilde{E})$ is positive Floquet exponent of $\text{Lib}_{\tilde{E}}$.

In the case $m = 0$ Theorem 1 was proved, first, in [4] when γ_0 is a straight line $x_2 = 0$, and then in [1],[2] in full generality (see also [6]). We want to show that passing to an arbitrary $m > 0$ is quite simple.

Sketch of proof: We express (6) with the instanton phase ($E = 0$). The tunnel WKB approximation for the normalized quasimodes reads

$$u_{L/R} = h^{-\frac{m+1}{2}} A_{L/R}(x) e^{-\frac{S_{L/R}}{h}} (1 + \mathcal{O}(h)),$$

where $S_{L/R} = d_0(x, a_{L/R})$ (distance along the instanton), and the amplitudes $A_{L/R}$ are solution of the transport equation

$$A(\lambda_1(2m+1) + \lambda_2 - \Delta S) + 2\nabla A \nabla S = 0. \quad (9)$$

Inserting it into (??) and applying asymptotic stationary phase, we obtain:

$$\Delta E_m \sim 4h^{\frac{1}{2}-m} \sqrt{\pi} D^{-\frac{1}{2}} A_L^2(x_0) P_0 e^{-\frac{S_0}{h}},$$

where $x_0 = x_E|_{E=0}$, $D = \frac{\partial^2 S_L}{\partial x_2^2}(x_0)$; $P_0 = \frac{\partial S_L}{\partial x_1}(x_0)$, and $S_0 = 2S_L(x_0)$.

From now on $\alpha \sim \beta$ means $\alpha = \beta(1 + o(1))$ as $h \rightarrow 0$, and also we omit subscripts L/R .

To find $A(0)$ we shall solve the first transport equation (??) along the instanton $x = \gamma_0(t)$. Putting $b(t) = A(\gamma_0(t))$, we get $b(0) = e^{-\omega_1 m t} \mathcal{J}(t) b(t)$, where

$$\mathcal{J}(t) = \exp \int_0^t \left(\frac{\Delta S}{2} - \frac{\lambda_1 + \lambda_2}{2} \right) dt.$$

On the other hand, we can use harmonic oscillator approximation for $b(t)$ as $t \rightarrow \infty$. Therefore

$$b(t) \sim \frac{\sqrt[4]{\lambda_1^{1+2m} \lambda_2 2^{\frac{m}{2}}}}{\sqrt{m!} \pi} (\xi_1(t))^m, \quad t \rightarrow +\infty$$

where $\xi_1(t)$ is a ξ_1 -coordinate of $\gamma_0(t)$.

Defining $\sigma = \lim_{t \rightarrow +\infty} e^{\lambda_1 t} \xi_1(t)$ and $\mathcal{J} = \mathcal{J}(+\infty)$ we see that

$$\Delta E_m \sim \frac{2^{m+2} h^{\frac{1}{2}-m}}{m! \sqrt{\pi} D^{\frac{1}{2}}} \sqrt{\lambda_1^{2m+1} \lambda_2} \sigma^{2m} \mathcal{J}^2 P_0 e^{-\frac{S_0}{h}}. \quad (10)$$

Let now S_E be a half of the action along Lib_E . In [1] we proved:

$$S_E - S_0 = \frac{E}{2\lambda_1} (1 + \log 2) + E T_E + o(E), \quad (11)$$

where T_E stands for time to move along γ_0 between the intersections with ∂U_E . Inserting (??) with $E(h) = h(1+2m)\lambda_1$ into (??), we get

$$\Delta E_m \sim \frac{2^{1-m} \sqrt{\pi} h \lambda_1}{m! e^{\frac{1}{2}+m} \pi} \mathcal{T} \rho^{2m+1} e^{-\frac{S_E}{h}},$$

where

$$\mathcal{T} = \mathcal{J}^2 \frac{P_0}{\lambda_1 \sigma} \frac{\sqrt{\lambda_2}}{\sqrt{D}}, \quad \rho = \frac{\sigma \sqrt{\lambda_1}}{\sqrt{h}} e^{-\lambda_1 T_E}.$$

One can easily see that $\rho \sim \sqrt{2m+1}$, hence

$$\Delta E_m \sim b_m \frac{h \omega_1}{\pi} \mathcal{T} e^{-\frac{S_{E(h)}}{h}}. \quad (12)$$

Thus, we arrived to the same formula as for $m = 0$, but for the numerical factor b_m . The rest of proof is similar to the case $m = 0$, its main ingredient is the following (see [2])

Proposition 2

$$\beta(E) = \lambda_2 - \frac{4 \log \mathcal{T}}{T(E)} (1 + o(1)),$$

where $T(E)$ denote the period of Lib_E .

Note that proof of this Proposition uses assumption $2\lambda_1 < \lambda_2$. When the instanton γ_0 is not a straight line, we resort to special coordinates (proposed in [7],[4]): s denotes arclength along γ_0 , while q is a coordinate along a normal to γ_0 . But these coordinates are ill-behaved when Euclidean curvature of γ_0 tends to infinity near $a_{L/R}$, which can happen, if $\frac{\lambda_2}{\lambda_1} \leq 2$.

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